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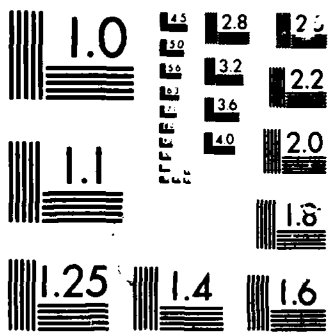
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US Army Corps
of Engineers
Construction Engineering

USA-CERL

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June 1986

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Computerization of the Preliminary Pollutant Limit Value Concept

by
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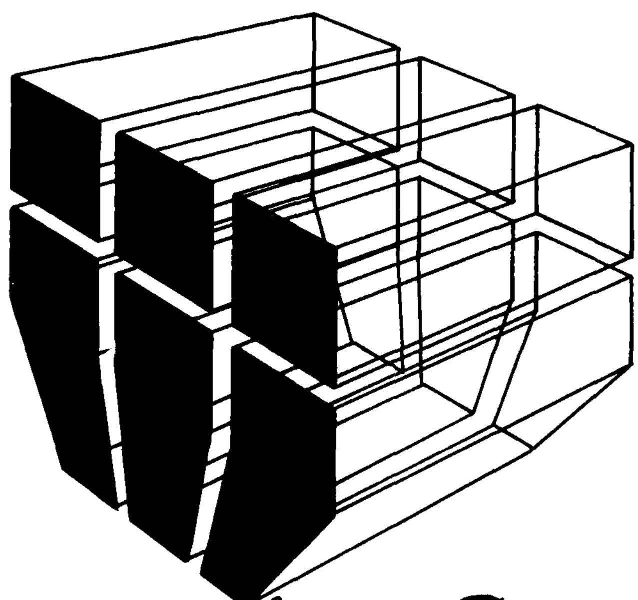

The Preliminary Pollutant Limit Value (PPLV) model developed by the U.S. Army Medical Bioengineering Research and Development Laboratory is an attempt to describe the environmental pathways through which humans may be exposed to toxic chemicals that have escaped into the environment. The model estimates the uptake/transformation of the compound at each step in each pathway, and arrives at a preliminary limit value in the environment for the compound of concern based on toxicological considerations. This report describes development of an interactive version of the PPLV model.

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The Preliminary Pollutant Limit Value (PPLV) model developed by the U.S. Army Medical Bioengineering Research and Development Laboratory is an attempt to describe the environmental pathways through which humans may be exposed to toxic chemicals that have escaped into the environment. The model estimates the uptake/transformation of the compound at each step in each pathway, and arrives at a preliminary limit value in the environment for the compound of concern based on toxicological considerations. This report describes development of an interactive version of the PPLV model.

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FOREWORD

This work was performed for the U.S. Army Medical Bioengineering Research and Development Laboratory (USAMBRDL) under Project Order 84PP4857. Dr. Mary Henry was the USAMBRDL Technical Monitor.

This research was performed by the Environmental Division (EN), U.S. Army Construction Engineering Research Laboratory (USA-CERL). Dr. R. K. Jain is Chief of EN. COL Paul J. Theuer is Commander and Director of USA-CERL, and Dr. L. R. Shaffer is Technical Director.

CONTENTS

COMPUTERIZATION OF THE PRELIMINARY POLLUTANT LIMIT VALUE CONCEPT

1 INTRODUCTION

Background

Regulatory limits for toxic chemicals in the environment are often set with respect to the level of the chemical that can be measured in the laboratory, rather than the actual toxicity of the compound. One reason for this practice is that making a connection between the acceptable daily dose to a human and the tolerable level in the environment is an extremely complex problem. This problem has been addressed in a theoretical model developed by the U.S. Army Medical Bioengineering Research and Development Laboratory (USAMBRDL). Called the Preliminary Pollutant Limit Value (PPLV) model, it is an attempt to describe the environmental pathways through which humans may be exposed to toxic chemicals that have escaped into the environment, estimate the uptake/transformation of the compound at each step in each pathway, and arrive at a preliminary limit value in the environment for the compound of concern based on toxicological considerations. This information is needed for responding to requirements of the Army Installation Restoration Program.

Objective

The objective of this effort was to provide an interactive version of the PPLV model, so that it can be easily tested and verified by a diverse Army user community. In addition, limited development of the data necessary to run the model was undertaken to aid in the model verification.

Approach

Data inputs required to run the model were defined and commercial chemical information systems were searched to obtain values for 303 chemicals of unique concern to the Army. Necessary characteristics of the interactive program were defined in conjunction with the sponsor, and software was designed to satisfy these requirements.

2 THE PPLV INTERACTIVE PROGRAM

The Model

USAMBRDL has developed and documented[1] the PPLV model to answer the following general question:

> Soil or water (or both) are contaminated with a chemical. If the land or water is intended to be used for one or more functions, what concentration of the chemical should be allowed to remain?

The user is expected to approach the model with one or more scenarios in mind. Based upon these scenarios, one or more of the pathways by which humans may be exposed to the pollutant through ingestion or inhalation are chosen. These pathways can be written like this:

1. water → human
2. soil → water → human
3. water → fish → human
4. soil → water → fish → human
5. water → crops → human
6. soil → water → crops → human
7. water → crops → livestock → human
8. soil → water → crops → livestock → human
9. water → livestock → human
10. soil → water → livestock → human
11. soil → vegetables → human
12. soil → plants → livestock → human

---

[1] Mitchell J. Small, *The Preliminary Pollutant Value Approach: Procedures and Database*, Technical Report 8210 (USAMBRDL, June 1984).

13. soil → plants → livestock → dairy products → human

14. soil → human

15. dust → human

16. soil → vapor → human

The pathways are treated as a series of environmental compartments, each containing the pollutant at equilibrium. The last compartment involves transfer of the pollutant to humans, which is considered to be a nonequilibrium process occurring at an assumed rate. The PPLV is the result of calculating back from the acceptable daily dose to the human in the last compartment through the pervious compartments until the tolerable concentration of pollutant in the first compartment is reached.

After the appropriate pathways are chosen, the data required for computations must be identified. From these data, a value for each pathway is calculated separately; this is called the Single Pathway Preliminary Pollutant Limit Value or SPPPLV. SPPLV equations have two general forms. If the chemical reaches humans without an intermediate compartment (such as direct ingestion of contaminated water), the form is

$$Cxi = IFi \times Dt \qquad \text{[Eq 1]}$$

where Cxi = the SPPLV for media X and pathway i
IFi = intake factor for pathway i
Dt = acceptable daily dose to human.

If the pathway contains one or more intermediate compartments, the SPPPLV equation takes the form:

$$Cxi = IFi \times Dt/Ki \qquad \text{[Eq 2]}$$

where Ki = composite partition coefficient for pollutant transfer.

Specific equations for Cxi and Ki for the 16 pathways described above are shown in Appendix A; a complete list of notation is given in Appendix B. More detailed explanations of the model can be found in:

1. Rosenblatt, D.H.; Dacre, J.C.; Cogley, D.R.; "An Environmental Fate Model Leading to Preliminary Pollutant Limit Values for Human Health Effects," *Environmental Risk Analysis for Chemicals*, R.J. Conway ed. (Van Nostrand Reinhold Co., 1980.)

2. Mitchell J. Small, *The Preliminary Pollutant Value Approach: Procedures and Database*, Technical Report 8210 (USAMBRDL, June 1984).

3. Rosenblatt et al., "Preliminary Pollutant Limit Values for Human Health Effects," *Environmental Science and Technology*, Vol 15, Number 7 (July 1980).

The System

A pilot system has been developed to grind through the pathway equations in Appendix A and to access and use the data stored on-line for a limited number of chemical compounds. The result is SPPPLVs for each pathway chosen, and a final PPLV for the whole scenario, which is obtained by normalizing the SPPPLVs. The PPLV pilot program is available as an experimental subsystem of the Environmental Technical Information System (ETIS).[2] ETIS can be accessed over WATS, Telenet, and commercial telephone lines by almost any kind of computer terminal. ETIS is an interactive, user-friendly system that can be used by people unfamiliar with computers.

Accessing ETIS

A user wishing to access the PPLV model after interactively entering ETIS need only transfer into the program. The following paragraphs provide instructions for accessing ETIS information by remote terminal.

After a log-in and a password have been acquired from USA-CERL's Environmental Division, ETIS can be accessed by following the directions in USA-CERL Technical Report N-56[3], DA Pamphlet 200-2[4], and USA-CERL Technical Report N-43[5]. After acquiring a remote terminal, a modem and a telephone line, dial the system's number (217/333-5067; WATS 800/637-0958). If there is no answer, the entire system is down

[2] R. D. Webster, et al., *Development of the Environmental Technical Information System*, Interim Report E-52/ADA 009668 (U.S. Army Construction Engineering Research Laboratory [USA-CERL], 1975).

[3] J. van Weringh, J. Patzer, R. Welsh, and R. Webster, *Computer-Aided Environmental Legislative Data System (CELDS) User Manual*, Technical Report N-56/ADA061126 (USA-CERL, 1978).

[4] *The Economic Impact Forecast System–Description and User Instructions*, DA PAM 200-2 (Department of the Army, December 1976).

[5] S. E. Thomas, et al., *Computer-Aided Environmental Impact Analysis for Industrial Procurement, and Research, Development, Test, and Evaluation Activities User Manual*, Technical Report N-43/ADA056997 (USA-CERL, June 1978).

for maintenance. Upon hearing a steady tone, connect the terminal/modem to the ETIS system as indicated in the manufacturer's instructions. After the correct name and password are entered, system messages will be displayed. Type "etis" at the prompt to start the system.

Keep several things in mind when using the system. The symbol <cr> used in some instructions means to depress the carriage return button. The instruction to type CTRL-d means to simultaneously depress the button marked CTRL and the letter d. An input error can be corrected by typing CTRL-h (hitting the CTRL and h buttons simultaneously) if the return button has not yet been depressed. This procedure will back the carriage up one space each time it is repeated. This can be done as many times as necessary. Every symbol which has been backspaced over has been removed from the terminal memory. Therefore, if the first digit of a six-digit number has been mistyped, you must depress CTRL-h six times and then retype all six digits. The corrected symbols will be overprinted on the paper or screen. To stop a long listing depress the button marked DEL (delete).

Using the PPLV Subsystem

When the system is started up, the following menu appears:

Options:

[1] Select Pathways

[2] Run Model

[3] Exit Model

The user must first choose one or more pathways over which the model will be run. This is done by choosing option 1 and then designating the desired pathways, as described above, by their assigned numbers. When all relevant pathways have been selected, a blank line is input by pressing the return key to indicate that the selection process is complete.

At this point, the model can be run by choosing option 2. The program will prompt the user for the pieces of data necessary to calculate the pollutant partition coefficients (Ki) and the SPPPLVs (Cxi) for each pathway chosen in option 1. If a piece of input data is unknown, the user can type a question mark to search the on-line database. The program then prompts for the Chemical Abstracts Service (CAS) registry number of the pollutant to perform the search. The database is exhaustively searched for all the occurrences of that CAS number, and all data values found are returned to the user along with the source of the data. At this point, the user can accept one of those values for use in continuing with the model run, or input a different value of his/her own choosing.

As the pollutant partition coefficients are calculated from the input data, they are shown to the user to be accepted or rejected. Acceptance is indicated by pressing the return key. Rejection is indicated by typing in a different value after the colon; this value is then used in all subsequent calculations. There is also a certain amount of default data built into the program for parameters such as body weight, weight of meat, fish, liquids taken per day, etc. Acceptance and rejection of this data is indicated the same way.

Once a particular piece of input data has been chosen or once a partition coefficient has been calculated, that value is used in all subsequent SPPPLV equations in which it occurs. This forces any one run of the model to be internally consistent. When all the necessary data has been collected from the user, the SPPPLVs are calculated and the equations are displayed for each pathway, and the final PPPLV is presented. The program then restarts itself at the option menu above.

While most of the program is menu-driven, with the user being prompted from step to step, there are three commands that can be used in response to each prompt. These are "?" to search the on-line database, "bye" to leave the system at any point, and "help" to see a short explanation of the data parameter being prompted for.

A sample session with the PPLV program over a few pathways is shown below. User responses are underlined.

Welcome to the PPLV Predictive Model

Options:

[1] Select Pathways

[2] Run Model

[3] Exit Model

Pathways selected: <u>none</u>.

Enter Option Number: <u>1</u>

Type in the number(s) of the pathway(s) you want to consider.

Type '?' to view pathways.

Type 'all' to consider all pathways.

Press <Return> key alone to stop selecting pathways.

pathway #: ?

The available pathways are:

1. water → human
2. soil → water → human
3. water → fish → human
4. soil → water → fish → human
5. water → crops → human
6. soil → water → crops → human
7. water → crops → livestock → human
8. soil → water → crops → livestock → human
9. water → livestock → human
10. soil → water → livestock → human
11. soil → vegetables → human
12. soil → plants → livestock → human
13. soil → plants → livestock → dairy products → human
14. soil → human
15. dust → human
16. soil → vapors → human

pathway #: 1

pathway #: 4

pathway #: 10

pathway #: (return key is pressed to indicate selection is complete)

You have selected:

Pathway 1: water → himan

Pathway 4: soil → water → fish → human

Pathway 10: soil → water → livestock → human

Do you want to change this list? (y or n): n

Options:

[1] Select Pathways

[2] Run Model

[3] Exit Model

Pathways selected: 1 4 10

Enter Option Number: 2

Enter value for Dt in mg/kg/day: ?

Enter CAS Registry Number: 608-93-5

1. 0.016 EPA (est.by Small 1984 from NWQCD) pentachlorobenzene

Do you want to use the above value for Dt in mg/kg/day? (y or n): y

Dt = 0.016 mg/kg/day

Adult body weight (Bw) = 70 kg: <cr>

Weight of fluids consumed = 1.6 liters/day: <cr>

Weight of fish consumed (Wf) = 0.02: .04

Foc is the fraction of organic carbon in soil.
Enter Foc: .21

There are 2 equations for estimation of soil organic carbon coefficient (Koc):

1. Koc = antilog (−0.55 * log Csol + 3.64)
   where Csol = Solubility of compound in water.

2. Koc = antilog (0.544 * log Kow + 1.38)
   where Kow = octanol/water partition coefficient.

Enter equation number: 1

Enter solubility of compound in water in mg/liter: 55

Koc = antilog (−0.55 * log Csol + 3.04)
  = antilog (−0.55 * log 55 + 3.04)
  = 8.026917 mg/kg in soil organic carbon per mg/liter in water: <cr>

Ksw is the pollutant partition coefficient between soil & water.
Ksw = 1/(Foc * Koc)
  = 1/(0.21 * 8.026917)
  = 0.593242 mg/liter in water per mg/kg in soil: <cr>

Kwf is pollutant partition coefficient between water & fish.

There are 2 equations for estimation of Kwf:

1. Kwf = Fish Bioconcentration Factor (BCF)

2. Kwf = antilog (0.76 * log Kow − 0.23)
   where: Kow = octanol/water partition coefficient.

Enter equation number: 2

Enter value for Kow: 4

Kwf = antilog (0.76 * log Kow − 0.23)
  = antilog (0.76 * log 4 + 0.23)
  = 1.25554: <cr>

Weight of human consumption of meat (Wa) = 0.21 kg/day: .11

Kwa is pollutant partition coefficient between water & bulk animal.

There are 2 equations for estimation of Kwa:

1. Kwa = Fa * antilog (−1.476 + 0.495 log Csol)

2. Kwa = Fa * antilog (−3.457 −0.5 log Kow)
   where: Fa = fraction of fat in livestock.
   Csol = solubility of compound in water.
   Kow = octanol/water partition coefficient.

Enter equation number: 1

Fraction of fat (Fa) in cattle = 0.3, in swine = 0.5

Enter value for Fa: .4

Kwa = Fa * antilog (−1.476 + 0.495 log Kwa)
  = 0.4 * antilog (−1.476 + 0.495 log 55)
  = 0.21636 mg/kg in animal per mg/liter in water: <cr>

Cw1 = (Bw/Ww) * Dt = 70 / 1.6 * 0.016 = 0.7
Cs2 = [(Bw/Wf) / (Ksw * Kwf)] * Dt = [(70/0.04) / (0.593242 * 1.25554)] * 0.016 = 37.592016
Cs5 = [(Bw/Wa) / (Ksw * Kwa)] * Dt
  = [(70/0.11) / (0.593242 * 0.21636)] * 0.016
  = 79.326129

PPLV = 0.681301

<Return> key to continue

Options:

[1] Select Pathways

[2] Run Model

[3] Exit Model

Pathways selected: 1 4 10

Enter Option Number: 3

Goodbye from the PPLV Predictive Model . . . . .

Verification of the Model

As of this writing, the PPLV model has not been reviewed and accepted by the Surgeon General or the U.S. Environmental Protection Agency (USEPA). The interactive PPLV program provides a tool that makes the model easier to use and more accessible, but has in no way added to the theoretical basis of the model; the algorithms provided by the sponsor were not changed or refined. Acceptance of the model by the regulatory agencies will enhance the utility of the program to field personnel.

One matter for attention is calculation of the PPLV from the SPPPLVs. At present, both water and soil SPPPLVs are normalized into one final PPLV. The usefulness of this indicator in real field situations would be increased if the PPLV were calculated twice - once for water, normalizing all the water SPPPLVs and similarly for soil.

3 DATABASE DEVELOPMENT

Eight databases were developed to provide input to all 16 pathways of the model:

1. Dt–acceptable daily human dose, mg/kg/day

2. Kow–octanol/water partition coefficient, mg/liter in octanol per mg/liter in water

3. BCF–fish bioconcentration factor, mg/kg in fish per mg/kg in water

4. Csol–solubility of compound in water, mg/liter at 25 degrees C

5. SOC–soil organic carbon, grams/gram

6. MW–molecular weight, grams/gram-mole

7. Po–saturation vapor pressure, mm Hg at 25 degrees C

8. PBF–plant bioconcentration factor, mg/kg in plant per mg/kg in soil.

Four major commercial chemical information systems were searched for all the data fields listed above: HAZARDLINE, CIS (RTECS and OHMTADS), NLM (TDB and TOXLINE), and TOXNET. The results of these searches were downloaded to an IBM XT, reformatted, and uploaded to the Pyramid computer where the PPLV software resides. The pilot database consists of 303 compounds; 169 of these compounds were provided by USAMBRDL as being of prime concern. Another 134 compounds commonly used on Army installations were added to the original list.

Compounds for which no data whatsoever are available in these commercial systems include fog oil, infrared screening smoke, BDNPA-F, ball powder, NQ, nitrodiphenylamine, nitrosophenylamine, lead salicilate, lead resorcylate, TACOT, violet dye, red dye, green dye, toluidene red toner, parlon, strontium oxalate, condensate water, a number of amino-nitrotoluenes and nitro-methylphenyls, 1,5-dimethyl-2,4-dinitrobenzene, 4 nitrobenzonitrile, 4,6-dinitroaniline, 2,4-dinitrobenzoic acid, pink water, TAX, and 2-nitroglycerol.

A number of issues were encountered in database development. The primary one was the vast amount of data available and its relevance to the specific scenarios that the PPLV model addresses. This was particularly true in developing values for Dt, which is a necessary parameter for all pathways of the model. Dt can be calculated from a number of different values, including:

1. The OSHA threshold limit value (TLV) or time weighted-average (TWA) which is based on inhalation of the chemical.

2. The FDA's acceptable daily intake (ADI), which refers to consumption of the material and has been developed mostly for food additives. (USEPA is in the process of developing these values for other chemical compounds.)

3. The LD50, which varies as to route of exposure depending upon the specific experimental conditions under which it was calculated.

Currently, the PPLV system displays all data available for a compound and requests the user to choose one or input his/her own value. The value of Dt that should be chosen in any particular run of the model varies according to the pathways (and the 3 routes of exposure the pathways describe) that the user has chosen for that run. Forcing the user to choose a Dt value from those available assumes use of the model by a user community sensitive to these issues. Other data that suffer from this problem of relevance, though to a lesser extent, are the PBF, BCF, and SOC values.

A related issue is that of data reliability. While future refinements to the model could include some judgment of the reliability of each datum that is supplied, and from this an estimate of reliability of the final PPLV could be calculated, this type of task is best undertaken by a panel of toxicological experts.

Finally, data coverage in the commercial information systems averages less than 50 percent for any one system, as shown below. The searches were performed by CAS number, which identifies a specific chemical

compound. The number of hits refers to the fact that *some* information was found, though it may not have been complete or relevant to the PPLV model. Again, while future refinements to the model could include an automatic login to one of these systems so that the user could search for values for compounds that are not included as part of the PPLV database, no one system appears to include complete coverage of the types of chemicals of concern to Army users.

Vendor/ Database	# Hits in 303 searches	Percentage Found
CIS OHMTADS	60	20
CIS RTECS	131	44
NLM RTECS	128	43
NLM TOXLINE	97	32
TOXNET	100	33
HAZARDLINE	104	35

4 SUMMARY AND RECOMMENDATIONS

The preliminary Pollutant Limit Value model has been made accessible to the Army environmental community through an interactive program that is part of the Environmental Technical Information System. The program can be used to arrive at a tolerable environmental limit for a pollutant in the soil or water, given that the acceptable daily dose of the pollutant to humans is known. A small database containing the input parameters for 303 compounds underlies the program.

It is recommended that the issues involved in provision of reliable input data to the users be addressed before further development or refinement of the model itself.

APPENDIX A:

SPPPLV EQUATIONS

Equations

Pathway 1: water → human
$Cw1 = (Bw / Ww) * Dt$

Pathway 2: soil → water → human
$Cs1 = [(Bw / Ww) * Dt] / Ksw$
$Ksw = 1 / (Foc * Koc)$

Pathway 3: water → fish → human
$Cw2 = [(Bw / Wf) / Kwf] * Dt$
Kwf = Fish Bioconcentration Factor (BCF) –OR–
$Kwf = \text{antilog}\,(0.76 * \text{low Kow} - 0.23)$

Pathway 4: soil → water → fish → human
$Cs2 = [(Bw / Wf) / (Ksw * Kwf)] * Dt$

Pathway 5: water → crops → human
$Cw3 = [(Bw / Wp) / Kwp] * Dt$
$Kwp = Ksp / Ksw$

Pathway 6: soil → water → crops → human
$Cs3 = [(Bw / Wp) / (Ksw * Kwp)] * Dt$

Pathway 7: water → crops → livestock → human
$Cw4 = [(Bw / Wa) / (Kwp * Kpa)] * Dt$
$Kpa = Fa * \text{antilog}\,(-1.476 + 0.495 \log Csol)$ –OR–
$Kpa = Fa * \text{antilog}\,(-3.457 - 0.5 \log Kow)$

Pathway 8: soil → water → crops → livestock → human
$Cs4 = [(Bw / Wa) / (Ksw * Kwp * Kpa)] * Dt$

Pathway 9: water → livestock → human
$Cw5 = [(Bw / Wa) / Kwa] * Dt$

$Kwa = Fa * \text{antilog}\,(-1.476 + 0.495 \log Csol)$ –OR–
$Kwa = Fa * \text{antilog}\,(-3.457 - 0.5 \log Kow)$

Pathway 10: soil → water → livestock → human
$Cwf = [(Bw / Wa) / (Ksw * Kwa)] * Dt$

Pathway 11: soil → vegetables → human
$Cs6 = [(Bw / Wp) / Ksp] * Dt$
$Ksp = 6 * PBF$

Pathway 12: soil → plants → livestock → human
$Cs7 = [(Bw / Wa) / (Ksp * Kpa)] * Dt$

Pathway 13: soil → plants → livestock → dairy products → human
$Cs8 = [(Bw / Wd) / (Ksp * Kpa * Kad)] * Dt$
Kad = 1.44 for Arochlor
Kad = 1 for all other compounds

Pathway 14: soil → human
$Cs9 = (Bwc / Wsc) * Dt$

Pathway 15: dust → human
$Cs10 = [(Bw * 10\hat{6}) / (Css * RB') * (1.6 / Fw) * Dt$

Pathway 16: soil → vapors → human
$Cs11 = (Bw / RB') * (1 / Ksv) * Dt$
$Ksv = VDo * Ksw/Csol$
$Vdo = 1.64 * 10000 * Po * (MW / T)$;

Definition of Partition Coefficients

Ksw = pollutant partition coefficient between soil & water
Ksw = mg/liter in water per mg/kg in soil
= 1 / (Foc * Koc)
where Foc is the fraction of organic carbon in soil (dimensionless)
paths 2, 4, 6, 8, 10.

Koc = pollutant partition coefficient between soil organic carbon and water
Koc = mg/kg in soil organic carbon per mg/liter in water
2 equations: 1. $Koc = \text{antilog}(0.55 * \log Csol + 3.04)$ 2. $Koc = \text{antilog}(0.544 * \log Kow + 1.38)$
where Csol is the solubility of chemical in water, mg/liter and Kow is the octanol/water partition coefficient, mg/liter in octanol per mg/liter in water
paths 2, 4, 6, 8, 10

Kwf = pollutant coefficient between water & fish.
Kwf = mg/kg in fish per mg/liter in water.

2 equations 1. Kwf = BCF
BCF is the fish bioconcentration factor, mg/kg in mg/kg in fish per mg/liter in water
2. Kwf = antilog(0.76 * log Kow – 0.23)

paths 3, 4.

Kpa = pollutant partition coefficient between plant matter & bulk animal, mg/kg in animal per mg/kg in plant.

paths 7, 8.

Kwa = pollutant partition coefficient between water and bulk animal mg/kg in animal per mg/L in water.

paths 9, 10, 12, 13.

2 equations for Kpa & Kwa:
1. Kpa = Kwa = Fa * antilog(–3.457 + 0.5 log Kow)
2. Kpa = Kwa = Fa * antilog(–1.476 – 0.495 log Csol)
Fa = fraction of fat in livestock
= 0.3 cattle, 0.5 swine, .0037 cow's milk.

Kad = pollutant partition coefficient between dairy product and bulk animal.
mg/L in dairy product per mg/kg bulk animal

path 13.

Kad = 1.44 for Arochlor
= 1 for all other compounds

Ksv = pollutant partition coefficient between vapor & soil
mg/m^3 in air per mg/kg in soil

path 16.

Ksv = VDo * Ksw / Csol
VDo = saturation vapor density, mg/m^3
$VDo = 1.64 * 10^4 * Po * MW/T$
Po = vapor density, mmHg
MW = molecular weight, grams/gram-mole
T = temperature; default = 612 degrees Kelvin

Ksp = pollutant partition coefficient between soil and plant matter
mg/kg in plant per mg/kg in soil

paths 11, 12, 13.

Ksp = 6 * PBF
PBF = plant bioconcentration factor, mg/kg in plant per mg/kg in soil

Kwp = pollutant partition coefficient between water & plant matter
mg/kg in plant per mg/L in water.

paths 5, 6, 7, 8.

Kwp = Ksp/Ksw

APPENDIX B:

NOTATION

ADI	Acceptable Daily Intake, mg/kg/day
BW	Adult human body weight, kg
BWc	Child body weight, kg
BCF	Pollutant bioconcentration factor in fish, mg/kg fish per mg/L water
Csf	Soil PPLV, mg/kg
Csi	Soil SPPPLV for pathway 1, mg/kg**
Css	Dust concentration in air, mg/m^3
Cwf	Water PPLV mg/L
Cwi	Water SPPPLV for pathway i, mg/kg
Csol	Pollutant solubility limit in water, mg/L
CAS	Chemical Abstracts Service
Dt	Pollutant acceptable daily human dose, mg/kg/day
EPA	Environmental Protection Agency
Fa	Fraction of fat in livestock or dairy
Ff	Fraction of lipids in fish
Fw	Fraction of year during which dust can occur
Foc	Fraction of organic carbon in soil
Ki	Overall pollutant partition coefficient for pathway i, units vary
Kad	Pollutant partition coefficient between dairy and bulk animal, mg/L per mg/kg
Kih, KjK	Nonspecified pollutant partition coefficients
Koc	Organic carbon in soil-water partition coefficient, mg/kg in soil organic carbon per mg/L in water
Kow	Octanol-water partition coefficient, mg/L in octanol per mg/L in water
Kpa	Pollutant partition coefficient between plant matter and bulk animal, mg/kg in animal per mg/kg in plant
Ksp	Pollutant partition coefficient between soil and plant matter, mg/kg in plant per mg/kg in soil
Ksv	Pollutant partition coefficient between soil and vapor in soil-pores, mg/m^3 in air per mg/kg in soil
Ksw	Pollutant partition coefficient between soil and water, mg/L in water per mg/kg in soil
Kwa	Pollutant partition coefficient between water and bulk animal, mg/kg in animal per mg/L in water
Kwf	Pollutant partition coefficient between water and fish, mg/kg in fish per mg/L in water
Kwp	Pollutant partition coefficient between water and plant matter, mg/kg in plant per mg/L in water
Kwv	Pollutant partition coefficient between water and air, mg/m^3 air per mg/L water
LD50	Estimated one-time pollutant dose lethal to 50 percent of mammalian species, mg/kg
MW	Molecular weight, g/g-mole
Po	Vapor pressure, mm Hg
PBF	Plant bioconcentration factor of pollutant, mg/kg in plant per mg/kg in soil
PPLV	Preliminary Pollutant Limit Value, mg/kg soil or mg/L water

RB	Inhaled volume of air daily, m^3
RB′	Inhaled volume of air in 8 hours by workers, m^3
SOC	Soil organic carbon content, g/g
SPPPLV	Single pathway PPLV, mg/kg soil or mg/L water
T	Temperature, °K or °C
TLV	Threshold Limit Value, mg/m^3
USAMBRDL	U.S. Army Medical Bioengineering Research and Development Laboratory
VD	Vapor density corresponding to Cw <Csol in equilibrium with Cs, mg/m^3
VDo	Saturation vapor density, mg/m^3
Wa	Human consumption of meat, kg/day
Wd	Human consumption of dairy, L/day
Wf	Human consumption of fish, kg/day
Wi	Human consumption of matter in pathway i**
Wp	Human consumption of vegetables, kg/day
Wsc	Child ingestion of soil, kg/day
Ww	Human consumption of drinking water, L/day

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